RAMMOHAN COLLEGE
FACULTY ACADEMIC PROFILE

Name: Dr. Hasibul Beg
Department: Chemistry
Email: beghasibul@gmail.com
Academic Background: PhD, From Vidyasagar University.
Position: Assistant Professor
Awards/ Honours:
Research Interest: Computational Chemistry
Ongoing Project:
Research Guidance:
Selected Publications:

1. Excited state intramolecular proton transfer in 3-hydroxychromone: a DFT-based computational study. Sankarlal Ash , Sankar Prasad De , Hasibul Beg , Ajay Misra* *Molecular Simulation, Vol. 37, No. 11, September 2011, 914–922.*

2. Use of polarizability and chemical hardness to locate the transition state and the potential energy curve for double proton transfer reaction: A DFT based study, Hasibul Beg, Sankar Prasad De, Sankarlal Ash, Ajay Misra * , *Computational and Theoretical Chemistry 984 (2012) 13–18.*

3. Polarizability, chemical hardness and ionization potential as descriptors to understand the mechanism of double proton transfer in acetamide dimer, Hasibul Beg, Sankar Prasad De, Sankarlal Ash, Debasish Das, Ajay Misra *, *Computational and Theoretical Chemistry 1005 (2013) 1–8.*

4. Computation of polarizability, hyper-polarizability and hardness as descriptor for enol–keto tautomerizations of 2-hydroxy pyridines, Hasibul Beg, Debasish Das, Sankarlal Ash, Ajay Misra*, ***Computational and Theoretical Chemistry 1017 (2013) 200–207.***

5. Morphology directing synthesis of 1-pyrene carboxaldehyde microstructures and their photo physical properties, Gobinda Prasad Sahoo, Debasish Das, Partha Sarathi Sheet, Hasibul Beg, Guillermo Salgado-Mor´an , Ajay Misra*, ***RSC Adv., 2014, 4, 10903–10911.***

6. Polarizability, hardness and electrophilicity as global descriptors for intramolecular proton transfer reaction path , Sankarlal Ash , Hasibul Beg , Prativa Mazumdar , Guillermo Salgado-Morán , Ajay Misra*, *Computational and Theoretical Chemistry 1031 (2014) 50–55.*

7. Global Reactivity Descriptors Along The Double Proton Transfer Co-ordinate of 2-Hydroxy Pyridine Dimmers: A DFT Based Computational Study, H. Beg, D. Mandal , A. Misra*, *The SciTech, Journal of Science & Technology, Vol-4, Issue-1, 2015, p-28-39.*

8. Computation of global reactivity descriptors and first hyper polarisability as a function of torsional angle of donor–acceptor substituted biphenyl ring system, Debkumar Mandal, Rakesh Maity, Hasibul Beg, Guillermo Salgado-Morán , Ajay Misra*, *MolecularPhysics, 2017.*